Hexachloropropene

1888-71-7 🛭	TXSID7062039

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 5.08

Global applicability domain: Inside

Local applicability domain index: 9.55e-01

Confidence level: 8.41e-01

Nearest Neighbors from the Training Set

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1,4-Dibromobenzene Measured: 5.21 Predicted: 5.09

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Naphthalene Measured: 5.19 Predicted: 5.07

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1,3,5-Trichlorobenzene Measured: 4.85 Predicted: 5.06

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1,2,4-Trichlorobenzene

Measured: 4.95 Predicted: 5.06

Image not found

1,2,3-Trichlorobenzene

Measured: 5.19 Predicted: 5.00